ChemComm

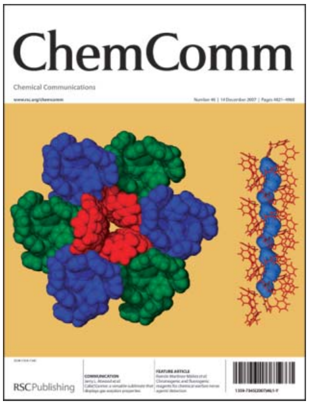
Chemical Communications

www.rsc.org/chemcomm

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www.rsc.org

IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (46) 4821–4960 (2007)



Cover
See Jerry L. Atwood *et al.*,
pp. 4848–4850.
Calix[5]arene sublimes to form a complex arrangement of independent helices, one of which is back-to-back and has gas sorption capabilities.
Image reproduced by permission of Scott J. Dalgarno, Jian Tian, John E. Warren, Thomas E. Clark, Mohamed Makha, Colin L. Raston and Jerry L. Atwood from *Chem. Commun.*, 2007, 4848.

CHEMICAL TECHNOLOGY

T89

Chemical Technology highlights the latest applications and technological aspects of research across the chemical sciences.

Chemical Technology

December 2007/Volume 4/Issue 12

www.rsc.org/chemicaltechnology

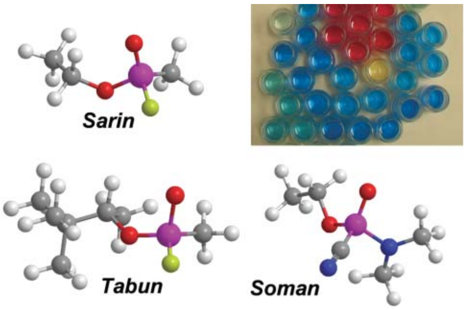
FEATURE ARTICLE

4839

Chromogenic and fluorogenic reagents for chemical warfare nerve agents' detection

Santiago Royo, Ramón Martínez-Máñez,* Félix Sancenón, Ana M. Costero,* Margarita Parra and Salvador Gil

New advanced chromo-fluorogenic concepts have recently been applied towards the development of optical systems for the easy detection of nerve agents and their simulants.



ChemComm

Chemical Communications

www.rsc.org/chemcomm

EDITORIAL STAFF

Editor
Sarah Thomas

Deputy editor
Kathryn Sear

Assistant editors
Emma Shiells, Alison Stoddart, Joanne Thomson, Kathleen Too, Jenna Wilson

Publishing assistants
Jackie Cockrill, Jayne Gough, Rachel Hegarty

Team leader, serials production
Helen Saxton

Technical editors
Celia Clarke, Nicola Convine, Alan Holder, Laura Howes, Sandra Jones, David Parker, Ken Wilkinson

Production administration coordinator
Sonya Spring

Administration assistants
Clare Davies, Donna Fordham, Julie Thompson

Publisher
Emma Wilson

Chemical Communications (print: ISSN 1359-7345; electronic: ISSN 1364-548X) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF. All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to RSC Distribution Services, c/o Portland Customer Services, Commerce Way, Colchester, Essex, UK CO2 8HP. Tel +44 (0)1206 226050; E-mail sales@rscdistribution.org

2007 Annual (print + electronic) subscription price: £1832; US$3462. 2007 Annual (electronic) subscription price: £1649; US$3116. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT. If you take an institutional subscription to any RSC journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip. Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank. Periodicals postage paid at Rahway, NJ, USA and at additional mailing offices. Airfreight and mailing in the USA by Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001, USA. US Postmaster: send address changes to Chemical Communications, c/o Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001. All despatches outside the UK by Consolidated Airfreight. PRINTED IN THE UK

© The Royal Society of Chemistry, 2007. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulations 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publisher or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA. The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions. Inclusion of an item in this publication does not imply endorsement by The Royal Society of Chemistry of the content of the original documents to which that item refers.

EDITORIAL BOARD

Chairman
Roeland J. M. Nolte, Nijmegen, The Netherlands
nolte@sci.kun.nl

Associate Editors
P. Andrew Evans, Liverpool, UK
andrew.evans@liverpool.ac.uk
Jonathan L. Sessler, Austin, USA
chemcommun@cm.utexas.edu
T. Don Tilley, Berkeley, USA
chemcomm@berkeley.edu

Scientific Editors
Alois Fürstner, Mülheim, Germany
fuerstner@mpi-muelheim.mpg.de
Mir Wais Hosseini, Strasbourg, France
hosseini@chimie.u-strasbg.fr

Members
Shankar Balasubramanian, Cambridge, UK
sb10031@cam.ac.uk
Penny Brothers, Auckland, New Zealand
p.brothers@auckland.ac.nz
Jillian M. Buriak, Edmonton, Canada
jburiak@ualberta.ca
Ben L. Feringa, Groningen. The Netherlands
feringa@chem.rug.nl
David Haddleton, Warwick, UK
D.M.Haddleton@warwick.ac.uk
Peter Kündig, Geneva, Switzerland
Peter.Kundig@chiorg.unige.ch
Nazario Martín, Madrid, Spain
nazmar@quim.ucm.es
Keiji Maruoka, Kyoto, Japan
maruoka@kuchem.kyoto-u.ac.jp
Ryong Ryoo, Taejon, Korea
rryoo@kaist.ac.kr
Ferdi Schüth, Mülheim, Germany
schueth@mpi-muelheim.mpg.de
Nicholas J. Turner, Manchester, UK
nicholas.turner@manchester.ac.uk

ADVISORY BOARD

Varinder Aggarwal, Bristol, UK
Frank Allen, CCDC, Cambridge, UK
Jerry L. Atwood, Columbia, USA
Amit Basak, Kharagpur, India
Dario Braga, Bologna, Italy
Xiao-Ming Chen, Guangzhou, China
Derrick Clive, Alberta, Canada
Marcetta Darensbourg, College Station, USA
Scott E. Denmark, Urbana, USA
Shaojun Dong, Changchun, China
Chris Easton, Canberra, Australia
Gregory C. Fu, Cambridge, USA
Tohru Fukuyama, Tokyo, Japan
Lutz Gade, Heidelberg, Germany
Philip Gale, Southampton, UK
George W. Gokel, St Louis, USA
Trevor Hambley, Sydney, Australia
Craig Hawker, Santa Barbara, USA
Andrew B. Holmes, Melbourne, Australia
Amir Hoveyda, Boston, USA
Steven M. Howdle, Nottingham, UK
Taeghwan Hyeon, Seoul, Korea
Biao Jiang, Shanghai, China
Karl Anker Jørgensen, Aarhus, Denmark
Kimoon Kim, Pohang, Korea
Susumu Kitagawa, Kyoto, Japan
Shu Kobayashi, Tokyo, Japan
Jérôme Lacour, Geneva, Switzerland
Teck-Peng Loh, Singapore
Tien-Yau Luh, Taipei, Taiwan
Doug MacFarlane, Monash, Australia
David MacMillan, Princeton, USA
Seth Marder, Atlanta, USA
Ilan Marek, Haifa, Israel
E. W. 'Bert' Meijer, Eindhoven, The Netherlands
Achim Müller, Bielefeld, Germany
Catherine Murphy, South Carolina, USA
Atsuhiro Osuka, Kyoto, Japan
Ian Paterson, Cambridge, UK
Maurizio Prato, Trieste, Italy
C. N. R. Rao, Bangalore, India
Christopher A. Reed, Riverside, USA
Robin Rogers, Alabama, USA
Michael Sailor, San Diego, USA
Jonathan W. Steed, Durham, UK
Zhong-Qun Tian, Xiamen, China
Carsten Tschierske, Halle, Germany
Herbert Waldmann, Dortmund, Germany
Henry N. C. Wong, Hong Kong, China
Eiji Yashima, Nagoya, Japan

Advertisement sales: Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

♾ The paper used in this publication meets the requirements of ANSI/NISO Z39.48–1992 (Permanence of Paper).

Royal Society of Chemistry: Registered Charity No. 207890.

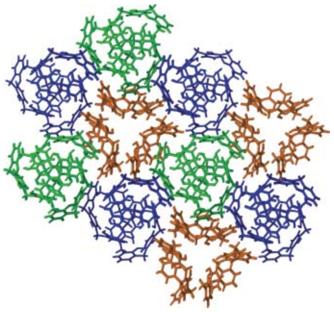
Authors may reproduce/republish portions of their published contribution without seeking permission from the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of The Royal Society of Chemistry.

4848

Calix[5]arene: a versatile sublimate that displays gas sorption properties

Scott J. Dalgarno, Jian Tian, John E. Warren, Thomas E. Clark, Mohamed Makha, Colin L. Raston and Jerry L. Atwood*

Sublimation of calix[5]arene affords two distinctly different polymorphs based on two different molecular conformations. In one, the calixarene packs in both 'self-included' and 'back-to-back' helical arrangements, the latter of which contains channels, rendering the polymorph active to sorption of CO_2 gas at STP.

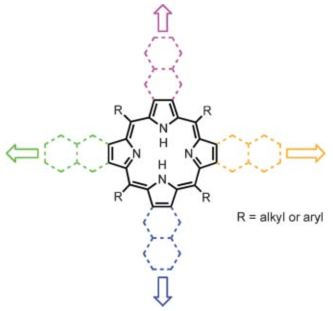


4851

A strategy for the stepwise ring annulation of all four pyrrolic rings of a porphyrin

Tony Khoury and Maxwell J. Crossley*

The repeated introduction of an α-dione unit and its reaction with an arene-1,2-diamine allows the stepwise annulation of all four pyrrolic rings of a porphyrin.

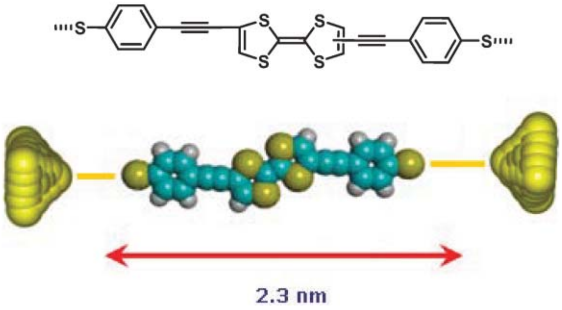


4854

Tetrathiafulvalene-based molecular nanowires

Francesco Giacalone, Mª Ángeles Herranz, Lucia Grüter, Mª Teresa González, Michel Calame, Christian Schönenberger, Carlos R. Arroyo, Gabino Rubio-Bollinger, Marisela Vélez, Nicolas Agraït* and Nazario Martín*

Electrical transport in a liquid environment has been demonstrated for a novel TTF-based molecular wire.

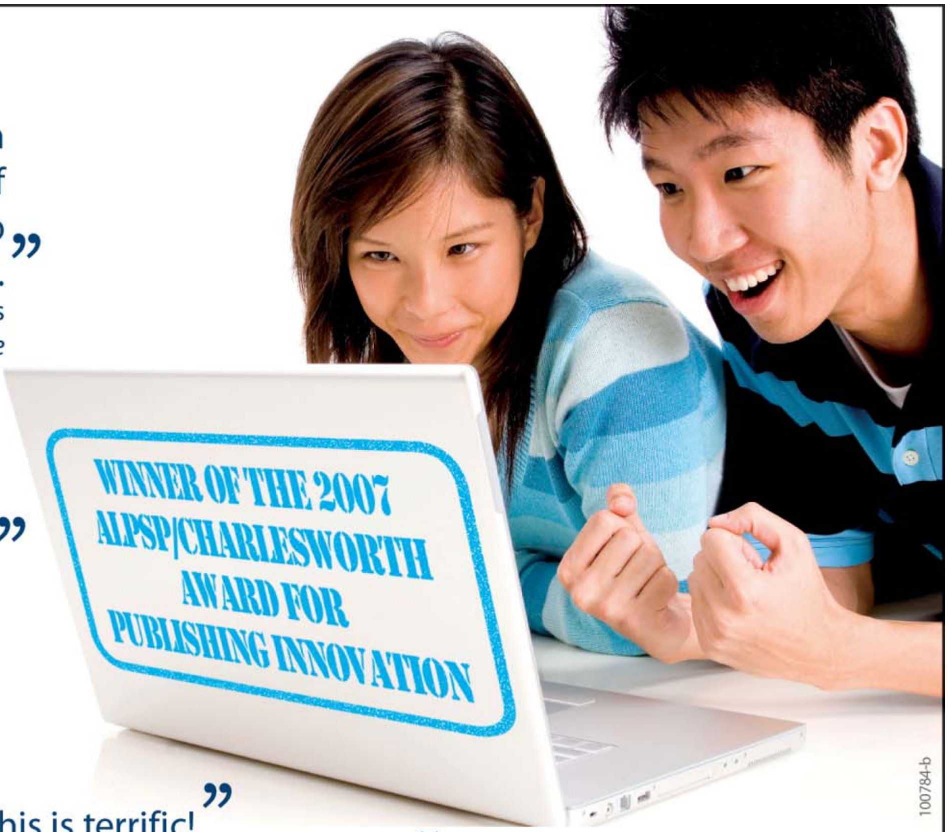


4857

Facile transformation of hydrophilic cellulose into superhydrophobic cellulose

Shenghai Li, Haibo Xie, Suobo Zhang* and Xianhong Wang

A facile method for constructing superhydrophobic cotton fabric has been developed by chemical vapor deposition (CVD). The CVD process is based on deposition of trichloromethylsilane from vapor-phase onto hydroxylated surfaces and subsequent hydrolyzation and polymerization to give uniform polymethylsiloxane coatings. The coating is also transparent so leading to no change in morphology and color of the cotton fabric.



“[Project Prospect] is an exciting application of ontologies that will help researchers.”
Midori Harris
European Bioinformatics Institute

“Invaluable for students.”
Stephen Haswell
University of Hull, UK

“This is terrific!”
Brian Shoichet
University of California, San Francisco and Molecular BioSystems' Board member

“…a fantastic resource for the community and a great use of the Gene Ontology and Sequence Ontology.”
Chris Mungall
Lawrence Berkeley National Laboratory

100784-b

Features include

Ontology terms linked to definitions and related papers
RSS feeds with ontology terms and compound structures
Hyperlinked compound information in text
IUPAC Gold Book terms linked

Benefits

Ideal for students
Completely free service
At a glance HTML view with additional features accessed by toolbox
Downloadable compound structures
Printer friendly

…with *Molecular BioSystems* and RSC Project Prospect

A revolutionary change in the way chemical and molecular biology articles are published is underway - thanks to RSC Project Prospect, an initiative developed by RSC Publishing together with academic partners. Not only can *Molecular BioSystems* readers click on named compounds in a journal article to download structures, more importantly they can link to definitions of ontology terms plus related papers. Powerful functionality instantly helps researchers and their students to find, understand and share (bio)chemical knowledge with each other quicker than ever before. See the science in *Molecular BioSystems* (and other RSC journals) come alive: visit the RSC Project Prospect website for more details plus examples.

RSC Publishing

www.projectprospect.org

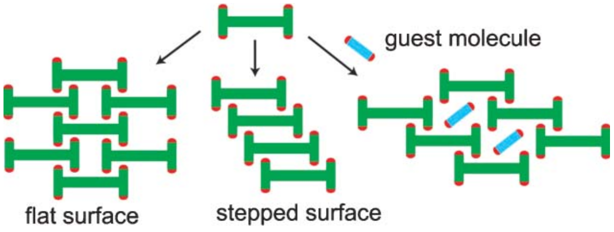
Registered Charity Number 207890

4860

Template-directed supramolecular self-assembly of coordination dumbbells at surfaces

Nian Lin,* Alexander Langner, Steven L. Tait, Chandrasekar Rajadurai, Mario Ruben* and Klaus Kern*

Unprecedented insight of template-directed supramolecular self-assembly. Scanning tunneling microscopy reveals, at single-molecular resolution, how external parameters re-direct the assembly of coordination supramolecules towards distinctive supramolecular organizations at a surface.

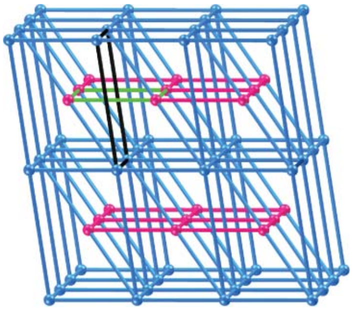


4863

An unprecedented (6,8)-connected self-penetrating network based on two distinct zinc clusters

Ya-Qian Lan, Xin-Long Wang, Shun-Li Li, Zhong-Min Su,* Kui-Zhan Shao and En-Bo Wang*

The first (6,8)-connected self-penetrating metal–organic framework has been constructed using an asymmetric neutral ligand based on dinuclear zinc clusters, as six-connected nodes, and trinuclear zinc clusters, as eight-connected nodes.

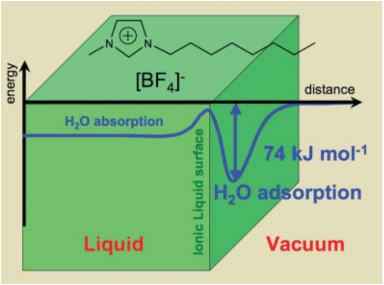


4866

Water adsorption on a liquid surface

Kevin R. J. Lovelock, Emily F. Smith, Alexey Deyko, Ignacio J. Villar-Garcia, Peter Licence and Robert G. Jones*

Monolayer adsorption of water onto an ionic liquid in ultra-high vacuum has been demonstrated, revealing a heat of adsorption which exceeds the heat of absorption into the bulk liquid by ≈40 kJ mol^{-1}.

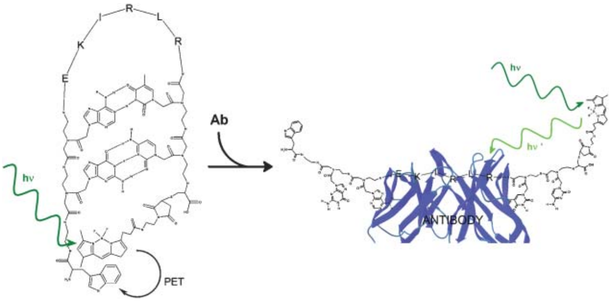


4869

Chimeric peptide beacons: a direct polypeptide analog of DNA molecular beacons

Kenneth J. Oh, Kevin J. Cash, Arica A. Lubin and Kevin W. Plaxco*

Described within is a new, polypeptide-based biosensor architecture, termed Chimeric Peptide Beacons (CPB). CPBs generate an optical output *via* a mechanism analogous to that employed in DNA-based molecular beacons and exhibit nanomolar detection limits as well as excellent target specificity.



Listen up
Speak out

chemistryworld

Your favourite monthly magazine invites you to go interactive

Chemistry World Podcast

The free monthly podcast from *Chemistry World* includes interviews and discussions on the latest topics in science: all in one bite sized chunk. Subscribe now at iTunes or download past and present podcasts directly from the *Chemistry World* website.

Chemistry World Blog
News, opinion & discussion

Got something to say? Then why not speak out on our new *Chemistry World* Blog: an interactive forum, updated daily, for the latest news, opinions and discussion about the chemical sciences. Why not post a question or comment on the science hitting the headlines.

RSC | Advancing the Chemical Sciences

www.chemistryworld.org

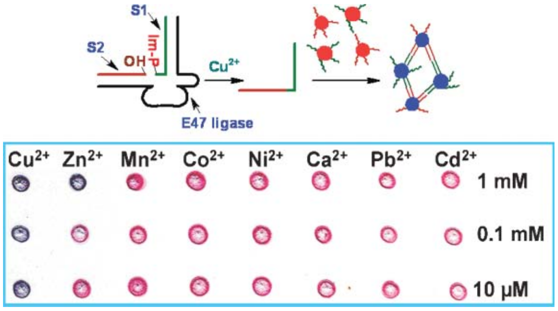
Registered Charity Number 207890

4872

Colorimetric Cu^{2+} detection with a ligation DNAzyme and nanoparticles

Juewen Liu and Yi Lu*

A highly sensitive and selective colorimetric sensor for Cu^{2+} was constructed using a ligation DNAzyme to assemble DNA-functionalized gold nanoparticles. Differing from cleavage based enzymes, ligation enzymes offer lower background.

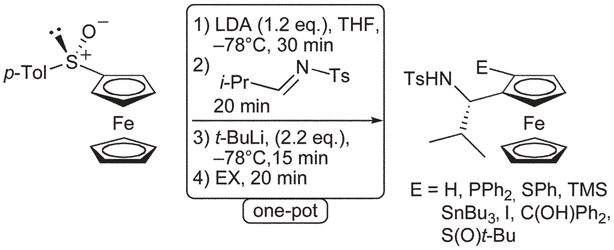


4875

A straightforward asymmetric synthesis of 1,2-disubstituted ferrocenylalkyl amines with the unusual (S_{Fc},*S*) configuration

Guillaume Grach, Jean-François Lohier,
Jana Sopkova-de Oliveira Santos, Vincent Reboul* and
Patrick Metzner*

A highly effective synthesis of rare 1,2-disubstituted ferrocenylalkyl amines with (S_{Fc},*S*) configuration has been achieved in a sequential one-pot methodology from (*S*)-*p*-tolylsulfinylferrocene.

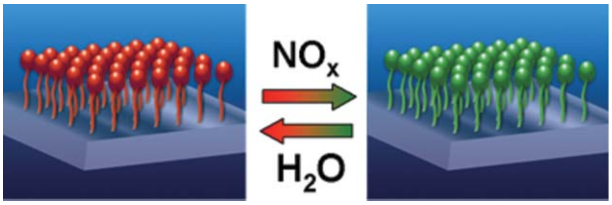


4878

Selective NO_x optical sensing with surface-confined osmium polypyridyl complexes

Antonino Gulino,* Tarkeshwar Gupta, Placido G. Mineo and Milko E. van der Boom*

Redox-active covalently bound monolayers undergo selective electron transfer with parts-per-million (ppm) levels of NO_2 and NO_x. This sensing device is read-out optically and reset with water.

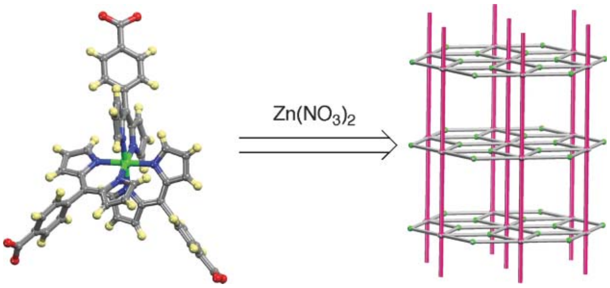


4881

Enantiopure *vs.* racemic metalloligands: impact on metal–organic framework structure and synthesis

Sergio J. Garibay, Jay R. Stork, Zhenqiang Wang, Seth M. Cohen* and Shane G. Telfer

Carboxylate-decorated tris(dipyrrinato) cobalt(III) complexes have been used to construct 2-D and 3-D metal–organic frameworks with infinite and trinuclear zinc secondary-building units.



Comprehensive and high quality coverage of multidisciplinary, international research relating to the measurement, pathways, impact and management of contaminants in all environments.

- Highly visible and cited in MEDLINE
- Accelerated publication rates, typically around 80 days
- Dedicated to the measurement of natural and anthropogenic sources of pollution with a view to assessing environmental and human health effects

Submit your work to JEM today

13080760

RSC Publishing

www.rsc.org/jem

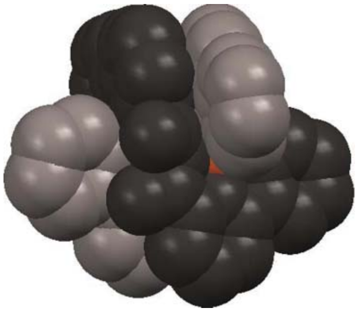
Registered Charity Number 207890

4884

Minimal structural reorganisation in the electrochemical oxidation of a dinuclear, double helical Cu(I) complex of a triazine-based pentadentate ligand

Elaine A. Medlycott and Garry S. Hanan*

The reversible reorganization in a Cu(I) double helicate of a new pentadentate triazine-containing ligand is investigated by electrochemical and crystallographic methods.

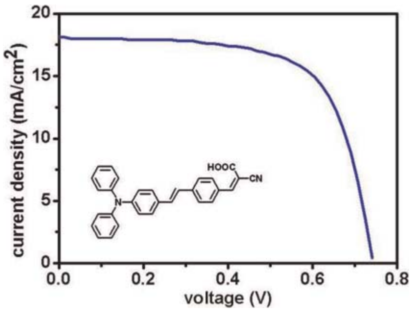


4887

A highly efficient organic sensitizer for dye-sensitized solar cells

Suyoung Hwang, Jung Ho Lee, Chanmoo Park, Hoinglae Lee, Chaekyu Kim, Chiyoung Park, Mi-Hyeon Lee, Wanin Lee, Jihee Park, Kyungkon Kim, Nam-Gyu Park* and Chulhee Kim*

A π-conjugated dye with donor–acceptor moieties exhibited high efficiency for a dye-sensitized solar cell.

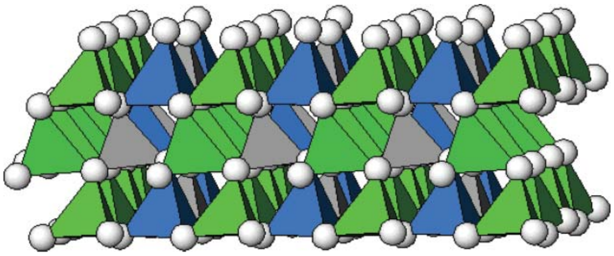


4890

The lithium intercalation compound Li_2CoSiO_4 and its behaviour as a positive electrode for lithium batteries

Christopher Lyness, Bruno Delobel, A. Robert Armstrong and Peter G. Bruce*

The electrochemical behaviour of three polymorphs of the lithium intercalation compound Li_2CoSiO_4, β_I, β_{II} and γ_0, as positive electrodes in rechargeable lithium batteries is investigated for the first time.

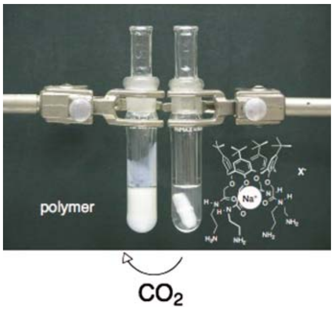


4893

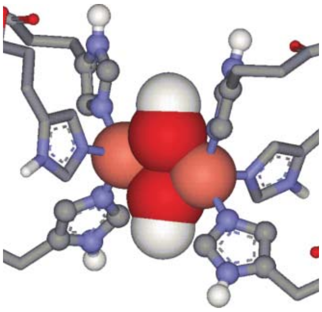
Using carbon dioxide and calix[4]arenes to separate sodium

Hexiang Zhang* and Dmitry M. Rudkevich

Reversible CO_2-induced precipitation of a calix[4]arene-based complex leads to selective separation of Na^+ salts.



4895

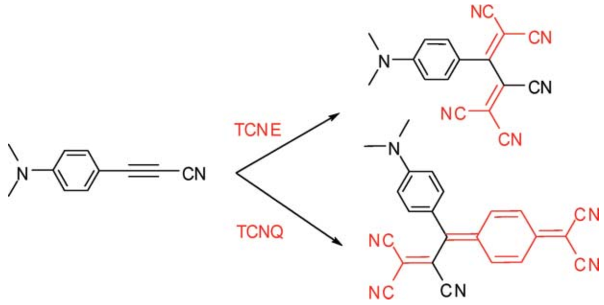


Scaffolded amino acids as a close structural mimic of type-3 copper binding sites

H. Bauke Albada, Fouad Soulimani, Bert M. Weckhuysen and Rob M. J. Liskamp*

For the first time we have demonstrated that scaffolded amino acids can be used as a close structural mimic of type-3 copper binding sites. Structural similarity is accessed by spectroscopic analysis of the Cu(II)-complex. Analysis of the CuO complex showed the presence of a $[TAC(HisAc)_3]_2Cu_2(OH)_2$ species. Oxygen binding and activation was shown by analysis of the bis(μ-hydroxo)dicopper(II)-complex and its reaction with a catechol.

4898

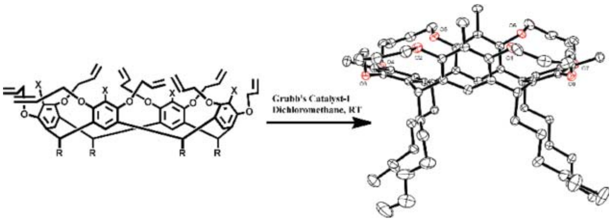


New strong organic acceptors by cycloaddition of TCNE and TCNQ to donor-substituted cyanoalkynes

Philippe Reutenauer, Milan Kivala, Peter D. Jarowski, Corinne Boudon, Jean-Paul Gisselbrecht, Maurice Gross and François Diederich*

The reaction of TCNE and TCNQ with acetylenes bearing an anilino donor and a cyano acceptor, followed by electrocyclic ring opening, led directly to new powerful electron acceptors that rival the benchmark reactants TCNE and TCNQ in their electron uptake capacity.

4901

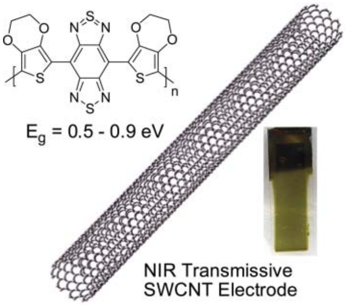


Synthesis of resorcin[4]arene cavitands by ring-closing metathesis

Sumedh N. Parulekar, Kirankirti Muppalla, Frank R. Fronczek and Kirpal S. Bisht*

The synthesis and X-ray crystal structures of the first resorcin[4]arene cavitands by ring-closing metathesis reaction are described.

4904



Low band gap EDOT–benzobis(thiadiazole) hybrid polymer characterized on near-IR transmissive single walled carbon nanotube electrodes

Timothy T. Steckler, Khalil A. Abboud, Matt Craps, Andrew G. Rinzler* and John R. Reynolds*

An electron donor/acceptor π-conjugated polymer composed of a bi-EDOT and benzobis(thiadiazole) repeat unit exhibits two reductions with a band gap ranging from ~0.5 to 0.8 eV depending on the method of band gap determination.

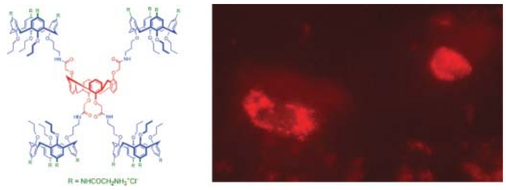
This journal is © The Royal Society of Chemistry 2007

4907

Efficient gene transfection with functionalised multicalixarenes

Ruth Lalor, Jessica L. DiGesso, Anja Mueller and Susan E. Matthews*

Novel amino functionalised multicalixarenes have been synthesised which show low cellular toxicity, effective DNA binding and, when featuring aliphatic amines, are efficient gene transfection agents.

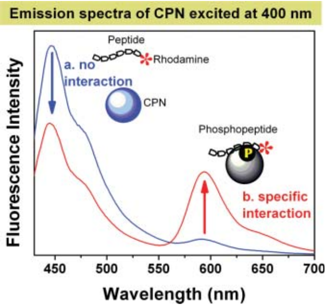


4910

Conjugated polymer nanoparticles for biochemical protein kinase assay

Joong Ho Moon,* Paul MacLean, William McDaniel and Lawrence F. Hancock*

Sensitive and reliable monitoring of kinase activity was reported by using highly efficient fluorescence resonance energy transfer of conjugated polymer nanoparticles (CPNs) to a rhodamine labelled peptide substrate.

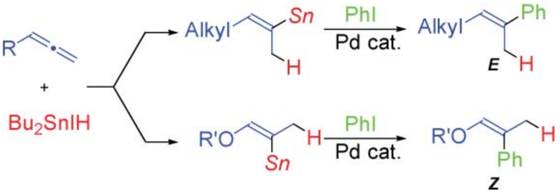


4913

Regio- and stereoselective hydrostannation of allenes using dibutyliodotin hydride (Bu$_2$SnIH) and successive coupling with aromatic halides

Naoki Hayashi, Kunazao Kusano, Shingo Sekizawa, Ikuya Shibata,* Makoto Yasuda and Akio Baba*

Regio- and stereoselective hydrostannation of allenes by using di-*n*-butyliodotin hydride (Bu$_2$SnIH) was accomplished to give α,β-disubstituted vinyltins, which induced the synthesis of multi-substituted alkenes in a one-pot procedure.

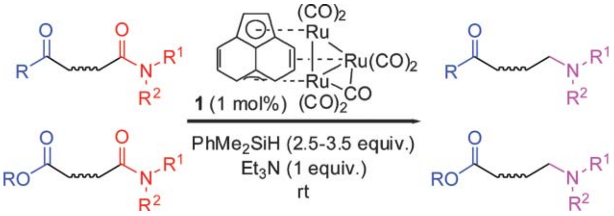


4916

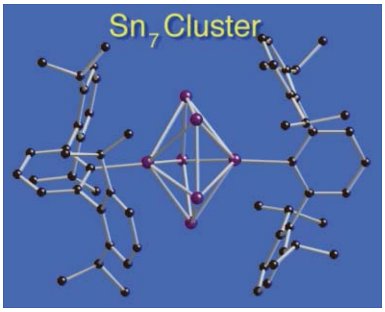
Functional group-selective poisoning of molecular catalysts: a ruthenium cluster-catalysed highly amide-selective silane reduction that does not affect ketones or esters

Hidehiro Sasakuma, Yukihiro Motoyama and Hideo Nagashima*

The addition of amines eliminates the catalytic activity of a triruthenium cluster in the hydrosilane reduction of ketones and esters without affecting the rate of reduction of amides; selective reduction of the amide group in amido ketones and amido esters is accomplished.



4919

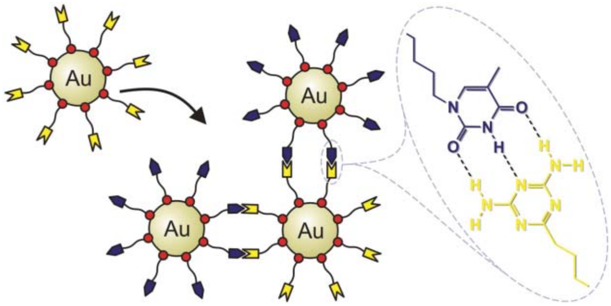


Convergent syntheses of [$Sn_7\{C_6H_3$-2,6-(C_6H_3-2,6-$^i Pr_2)_2\}_2$]: a cluster with a rare pentagonal bipyramidal motif

Eric Rivard, Jochen Steiner, James C. Fettinger, Jason R. Giuliani, Matthew P. Augustine and Philip P. Power*

Two complementary routes to an unusual pentagonal bipyramidal cluster, $Sn_5(SnAr')_2$ (Ar′ = terphenyl ligand), are reported.

4922

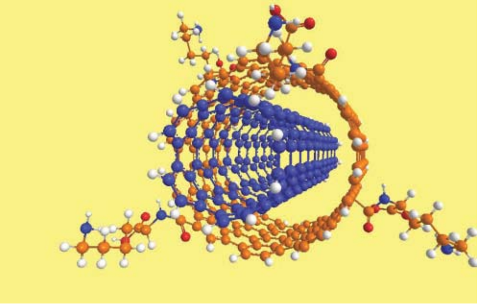


Selective co-aggregation of gold nanoparticles functionalised with complementary hydrogen-bonding groups

Coenraad R. van den Brom, Petra Rudolf, Thomas T. M. Palstra* and Bart Hessen*

Molecular recognition between two species of Au_{55} clusters bearing complementary hydrogen-bonding groups provides a facile route to accomplish solvent-controlled assembly of two-component 3D nanoparticle aggregates.

4925

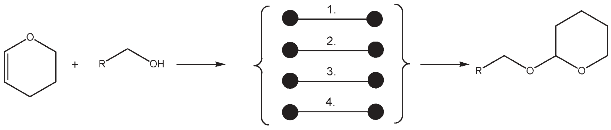


Amino acid functionalization of double-wall carbon nanotubes studied by Raman spectroscopy

Gabriele Marcolongo, Giorgio Ruaro, Marina Gobbo and Moreno Meneghetti*

Double-wall carbon nanotubes (DWNT) have been oxidized with MnO_4^- and then functionalized with lysine groups. Raman spectra show that the internal nanotubes are protected by the external ones during the strong oxidation and that the external ones have been functionalized.

4928



Parallel synthesis in an EOF-based micro reactor

Charlotte Wiles* and Paul Watts

We present herein a flexible micro reactor system that enables parallel syntheses to be performed under electroosmotic flow. Employing the synthesis, and deprotection, of THP ethers as model reactions, we were able to demonstrate for the first time the scale-out of EOF-based reactions. Using this approach, catalysts and reagents can be screened in parallel, offering time and costs savings compared to conventional batch reactors.

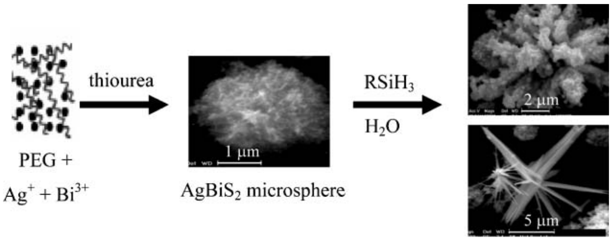
This journal is © The Royal Society of Chemistry 2007

4931

Synthesis of $AgBiS_2$ microspheres by a templating method and their catalytic polymerization of alkylsilanes

Jiaqiang Wang,* Xikung Yang, Wenbing Hu, Bin Li, Jiangmei Yan and Jinjin Hu

$AgBiS_2$ microspheres synthesized by using PEG as a template serve as active catalysts for the polymerization of an alkylsilane, $C_{18}H_{37}SiH_3$ with water to form silanols. This reaction takes place under relatively mild conditions (refluxing butanone).

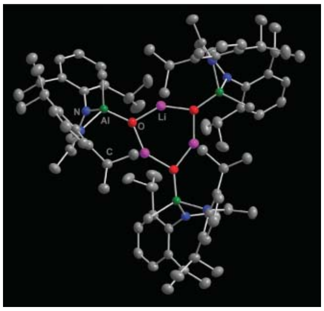


4934

Base free lithium-organoaluminate and the gallium congener: potential precursors to heterometallic assemblies

Sanjay Singh, Jianfang Chai, Aritra Pal, Vojtech Jancik, Herbert W. Roesky* and Regine Herbst-Irmer

Reactions of organo-aluminium and -gallium monohydroxide LMMe(OH) with $Li[N(SiMe_3)_2]$ afford the assembly of the heterobimetallic lithium-aluminate and -gallate $[LM(Me)OLi]_3$ (M = Al, Ga; L = $HC\{C(Me)N\text{-}2,6\text{-}iPr_2C_6H_3\}_2$) with the central six-membered Li_3O_3 core.

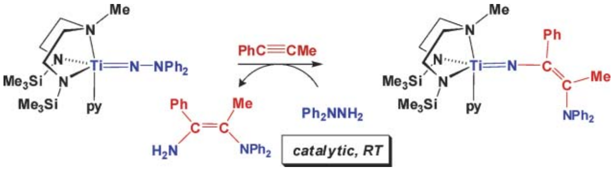


4937

New ligand platforms for developing the chemistry of the Ti=N–NR_2 functional group and the insertion of alkynes into the N–N bond of a Ti=N–NPh_2 ligand

Jonathan D. Selby, Catherine D. Manley, Marta Feliz, Andrew D. Schwarz, Eric Clot* and Philip Mountford*

New supporting ligand platforms for the terminal Ti=N–NR_2 functional group are described, along with the catalytic insertion of alkynes into the N–N bond of a titanium hydrazide ligand.

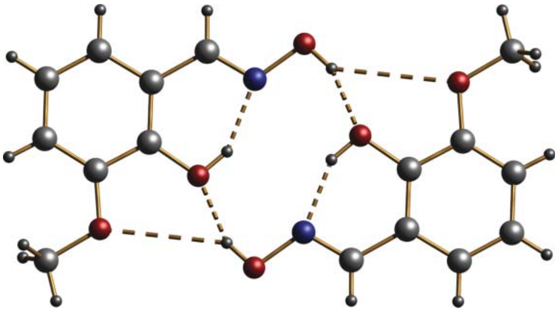


4940

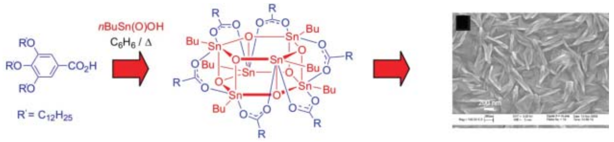
Supramolecular chemistry in metal recovery; H-bond buttressing to tune extractant strength

Ross S. Forgan, Peter A. Wood, John Campbell, David K. Henderson, Fiona E. McAllister, Simon Parsons, Elna Pidcock, Ronald M. Swart and Peter A. Tasker*

3-Substitution of salicylaldoximes facilitates significant changes in both their solid state cavity sizes and ability to extract copper. DFT and PIXEL calculations have shown that this is due primarily to the 3-substituent buttressing the stabilising *inter*ligand H-bonds.



4943

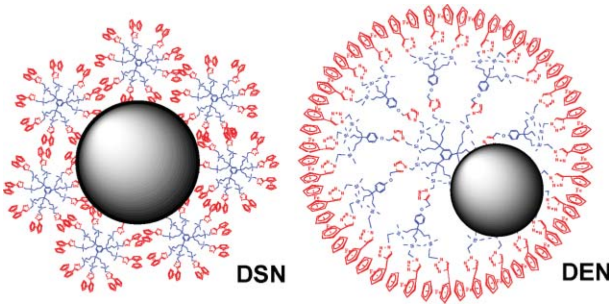


Modular construction and hierarchical gelation of organooxotin nanoclusters derived from simple building blocks

Uwe Hahn, Andrew R. Hirst, Juan Luis Delgado, Adrien Kaeser, Béatrice Delavaux-Nicot, Jean-Francois Nierengarten* and David K. Smith*

Tin-drum nanoclusters are demonstrated to be highly tunable, self-assembling modules which are capable of underpinning gel-phase nanomaterials.

4946

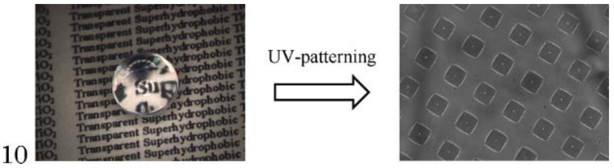


Catalytically efficient palladium nanoparticles stabilized by "click" ferrocenyl dendrimers

Cátia Ornelas, Lionel Salmon, Jaime Ruiz Aranzaes and Didier Astruc*

"Click" chemistry offers a unique way to cleanly provide heterocyclic ligands trapping metal species such as Pd(OAc)$_2$ in "click" dendrimers. Reduction using methanol yields catalytically efficient dendrimer-stabilized (DSN) or dendrimer-encapsulated Pd nanoparticles (DENs) depending on the dendrimer generation. The smallest Pd-DENs (1 nm), obtained with the 27-branch dendrimer, are the most active catalysts.

4949



A transparent and photo-patternable superhydrophobic film

Xintong Zhang, Hiroki Kono, Zhaoyue Liu, Shunsuke Nishimoto, Donald A. Tryk, Taketoshi Murakami, Hideki Sakai, Masahiko Abe and Akira Fujishima*

Transparent superhydrophobic TiO$_2$ films, prepared by spin-coating a TiO$_2$ slurry on glass substrates and modifying the resultant films with fluoroalkylsilane molecules, could be patterned with ultraviolet light, producing superhydrophobic/superhydrophilic surface micropatterns.

4952

Nornicotine-organocatalyzed aqueous reduction of α,β-unsaturated aldehydes

Andrew P. Brogan, Tobin J. Dickerson* and Kim D. Janda*

Under homogeneous aqueous conditions, the nicotine-derived natural product nornicotine has been found to catalyze the chemoselective reduction of α,β-unsaturated aldehydes.

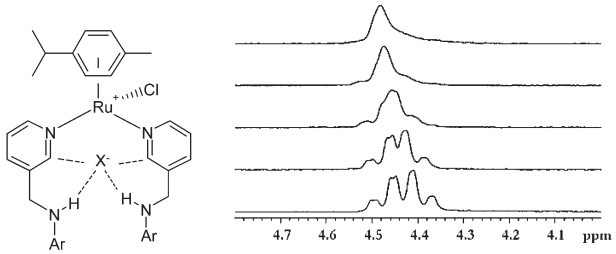
This journal is © The Royal Society of Chemistry 2007

4955

Anion binding in (arene)ruthenium(II)-based hosts

Sara Jane Dickson, Stefano C. G. Biagini and Jonathan W. Steed*

Asymmetric ruthenium(II) complexes of a flexible aminomethylpyridine derivative exhibit diastereotopic ligand methylene protons, as measured by NMR spectroscopy. Anion binding renders these protons magnetically equivalent, with the amount of anion needed to bring about magnetic equivalence correlating to the anion binding constant.



Save valuable time searching for that elusive piece of vital chemical information.

Let us do it for you at the Library and Information Centre of the RSC.

We are your chemical information support, providing:

- Chemical enquiry helpdesk
- Remote access chemical information resources
- Speedy response
- Expert chemical information specialist staff

Tap into the foremost source of chemical knowledge in Europe and send your enquiries to

library@rsc.org

RSC Publishing

www.rsc.org/library

12120515

AUTHOR INDEX

Abboud, Khalil A., 4904
Abe, Masahiko, 4949
Agraït, Nicolas, 4854
Albada, H. Bauke, 4895
Armstrong, A. Robert, 4890
Arroyo, Carlos R., 4854
Astruc, Didier, 4946
Atwood, Jerry L., 4848
Augustine, Matthew P., 4919
Baba, Akio, 4913
Biagini, Stefano C. G., 4955
Bisht, Kirpal S., 4901
Boudon, Corinne, 4898
Brogan, Andrew P., 4952
Bruce, Peter G., 4890
Calame, Michel, 4854
Campbell, John, 4940
Cash, Kevin J., 4869
Chai, Jianfang, 4934
Clark, Thomas E., 4848
Clot, Eric, 4937
Cohen, Seth M., 4881
Costero, Ana M., 4839
Craps, Matt, 4904
Crossley, Maxwell J., 4851
Dalgarno, Scott J., 4848
Delavaux-Nicot, Béatrice, 4943
Delgado, Juan Luis, 4943
Delobel, Bruno, 4890
Deyko, Alexey, 4866
Dickerson, Tobin J., 4952
Dickson, Sara Jane, 4955
Diederich, François, 4898
DiGesso, Jessica L., 4907
Feliz, Marta, 4937
Fettinger, James C., 4919
Forgan, Ross S., 4940
Fronczek, Frank R., 4901
Fujishima, Akira, 4949
Garibay, Sergio J., 4881
Giacalone, Francesco, 4854
Gil, Salvador, 4839
Gisselbrecht, Jean-Paul, 4898
Giuliani, Jason R., 4919
Gobbo, Marina, 4925
González, M^{a} Teresa, 4854
Grach, Guillaume, 4875
Gross, Maurice, 4898
Grüter, Lucia, 4854
Gulino, Antonino, 4878
Gupta, Tarkeshwar, 4878
Hahn, Uwe, 4943
Hanan, Garry S., 4884
Hancock, Lawrence F., 4910
Hayashi, Naoki, 4913
Henderson, David K., 4940
Herbst-Irmer, Regine, 4934
Herranz, M^{a} Ángeles, 4854
Hessen, Bart, 4922
Hirst, Andrew R., 4943
Hu, Jinjin, 4931
Hu, Wenbing, 4931
Hwang, Suyoung, 4887
Jancik, Vojtech, 4934
Janda, Kim D., 4952
Jarowski, Peter D., 4898
Jones, Robert G., 4866
Kaeser, Adrien, 4943
Kern, Klaus, 4860
Khoury, Tony, 4851
Kim, Chaekyu, 4887
Kim, Chulhee, 4887
Kim, Kyungkon, 4887
Kivala, Milan, 4898
Kono, Hiroki, 4949
Kusano, Kazunao, 4913
Lalor, Ruth, 4907
Lan, Ya-Qian, 4863
Langner, Alexander, 4860
Lee, Hoinglae, 4887
Lee, Jung Ho, 4887
Lee, Mi-Hyeon, 4887
Lee, Wanin, 4887
Li, Bin, 4931
Li, Shenghai, 4857
Li, Shun-Li, 4863
Licence, Peter, 4866
Lin, Nian, 4860
Liskamp, Rob M. J., 4895
Liu, Juewen, 4872
Liu, Zhaoyue, 4949
Lohier, Jean-François, 4875
Lovelock, Kevin R. J., 4866
Lu, Yi, 4872
Lubin, Arica A., 4869
Lyness, Christopher, 4890
MacLean, Paul, 4910
Makha, Mohamed, 4848
Manley, Catherine D., 4937
Marcolongo, Gabriele, 4925
Martín, Nazario, 4854
Martínez-Máñez, Ramón, 4839
Matthews, Susan E., 4907
McAllister, Fiona E., 4940
McDaniel, William, 4910
Medlycott, Elaine A., 4884
Meneghetti, Moreno, 4925
Metzner, Patrick, 4875
Mineo, Placido G., 4878
Moon, Joong Ho, 4910
Motoyama, Yukihiro, 4916
Mountford, Philip, 4937
Mueller, Anja, 4907
Muppalla, Kirankirti, 4901
Murakami, Taketoshi, 4949
Nagashima, Hideo, 4916
Nierengarten, Jean-Francois, 4943
Nishimoto, Shunsuke, 4949
Oh, Kenneth J., 4869
Ornelas, Cátia, 4946
Pal, Aritra, 4934
Palstra, Thomas T. M., 4922
Park, Chanmoo, 4887
Park, Chiyoung, 4887
Park, Jihee, 4887
Park, Nam-Gyu, 4887
Parra, Margarita, 4839
Parsons, Simon, 4940
Parulekar, Sumedh N., 4901
Pidcock, Elna, 4940
Plaxco, Kevin W., 4869
Power, Philip P., 4919
Rajadurai, Chandrasekar, 4860
Raston, Colin L., 4848
Reboul, Vincent, 4875
Reutenauer, Philippe, 4898
Reynolds, John R., 4904
Rinzler, Andrew G., 4904
Rivard, Eric, 4919
Roesky, Herbert W., 4934
Royo, Santiago, 4839
Ruaro, Giorgio, 4925
Ruben, Mario, 4860
Rubio-Bollinger, Gabino, 4854
Rudkevich, Dmitry M., 4893
Rudolf, Petra, 4922
Ruiz Aranzaes, Jaime, 4946
Sakai, Hideki, 4949
Salmon, Lionel, 4946
Sancenón, Félix, 4839
Sasakuma, Hidehiro, 4916
Schönenberger, Christian, 4854
Schwarz, Andrew D., 4937
Sekizawa, Shingo, 4913
Selby, Jonathan D., 4937
Shao, Kui-Zhan, 4863
Shibata, Ikuya, 4913
Singh, Sanjay, 4934
Smith, David K., 4943
Smith, Emily F., 4866
Sopkova-de Oliveira Santos, Jana, 4875
Soulimani, Fouad, 4895
Steckler, Timothy T., 4904
Steed, Jonathan W., 4955
Steiner, Jochen, 4919
Stork, Jay R., 4881
Su, Zhong-Min, 4863
Swart, Ronald M., 4940
Tait, Steven L., 4860
Tasker, Peter A., 4940
Telfer, Shane G., 4881
Tian, Jian, 4848
Tryk, Donald A., 4949
van den Brom, Coenraad R., 4922
van der Boom, Milko E., 4878
Vélez, Marisela, 4854
Villar-Garcia, Ignacio J., 4866
Wang, En-Bo, 4863
Wang, Jiaqiang, 4931
Wang, Xianhong, 4857
Wang, Xin-Long, 4863
Wang, Zhenqiang, 4881
Warren, John E., 4848
Watts, Paul, 4928
Weckhuysen, Bert M., 4895
Wiles, Charlotte, 4928
Wood, Peter A., 4940
Xie, Haibo, 4857
Yan, Jiangmei, 4931
Yang, Xikung, 4931
Yasuda, Makoto, 4913
Zhang, Hexiang, 4893
Zhang, Suobo, 4857
Zhang, Xintong, 4949

FREE E-MAIL ALERTS AND RSS FEEDS

Contents lists in advance of publication are available on the web *via* www.rsc.org/chemcomm – or take advantage of our free e-mail alerting service (www.rsc.org/ej_alert) to receive notification each time a new list becomes available.

Try our RSS feeds for up-to-the-minute news of the latest research. By setting up RSS feeds, preferably using feed reader software, you can be alerted to the latest Advance Articles published on the RSC web site. Visit www.rsc.org/publishing/technology/rss.asp for details.

ADVANCE ARTICLES AND ELECTRONIC JOURNAL

Free site-wide access to Advance Articles and electronic form of this journal is provided with a full-rate institutional subscription. See www.rsc.org/ejs for more information.

* Indicates the author for correspondence: see article for details.

Electronic supplementary information (ESI) is available *via* the online article (see http://www.rsc.org/esi for general information about ESI).

December 2007 / Volume 4 / Issue 12 / ISSN 1744-1560 / CTHEC2 / www.rsc.org/chemicaltechnology

Chemical Technology

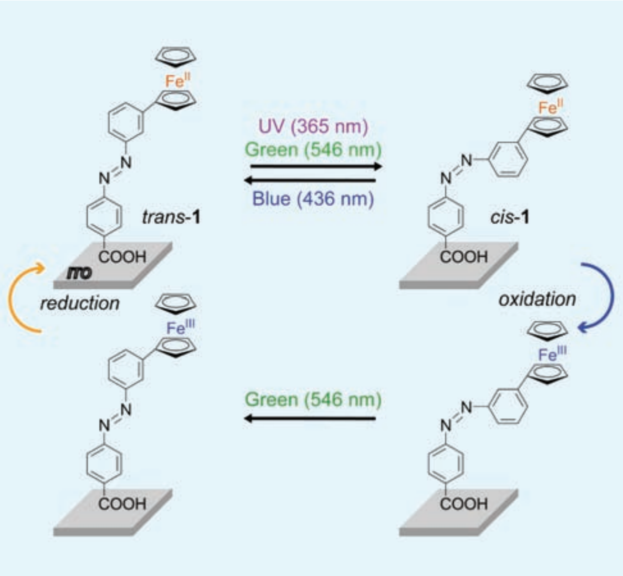
Only one light source required to swap isomers thanks to ferrocene

Mastering molecular memory

A molecule that switches shape when triggered by light could lead to nanoscale memory devices, say chemists in Japan.

Hiroshi Nishihara and colleagues from the University of Tokyo have combined photochemistry and electrochemistry to make a molecule that can be switched from one form to another, and then back again, using a single source of light. Previous such photochromic molecules have needed a second light source of a different wavelength to be flipped back to their original state.

'Focussing dual light sources on the same small spot can be a problem from the perspective of both technical difficulty and cost performance,' said Nishihara. 'Our system is the first monolayer film of photochromic molecules which can be reversibly switched by a single light source.'



The molecule flips between states using only green light

The Tokyo team used a photochromic molecule that incorporates an iron-containing ferrocene group, which they deposited in a single layer onto a transparent electrode surface. When the molecule's iron core is in the 2+ oxidation state, green light isomerises a double bond in the structure from *trans* to *cis*, changing the shape. When the iron is electrochemically converted to Fe(III), the same green light will convert *cis* form back to the *trans* isomer.

'This work takes one of the most challenging leaps for chemists: to interface small molecule materials with developing infrastructure from microtechnology,' said Amar Flood, who researches molecular switches at Indiana University, Bloomington, US. 'It is critical to take this step – chemists mustn't lose sight of engineering, because otherwise our engineering colleagues will lose sight of us.'

Nishihara is now working to fine-tune the chemical structure of the molecule, to increase the proportion of molecules in the sample that isomerise in response to the light. 'The other [project] is to immobilise the molecules onto submicron-sized electron arrays, to demonstrate high density memory device fabrication,' he said.

James Mitchell Crow

Reference

K Namiki *et al.*, *Chem. Commun.*, 2007, 4650 (DOI: 10.1039/b713107k)

In this issue

Detection at a distance

Spectroscopy measures atomic ratios to find explosives

Microbes fuel the way to better water treatment

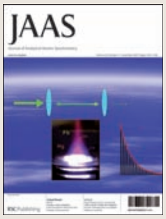
Bacteria act as miner's canary for toxin levels

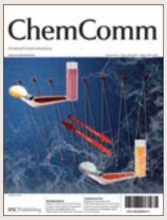
Interview: The fascination of catalysis

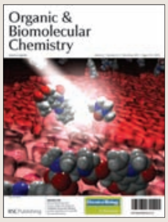
Ferdi Schüth talks to Madelaine Chapman about rockets, catalysis and law

Instant insight: Holographic data storage

Avtar Matharu and colleagues from the University of York, UK, explain how, when it comes to data, size matters







The latest applications and technological aspects of research across the chemical sciences

©The Royal Society of Chemistry 2007

Application highlights

Hydrogen and oxygen are evolved in separate streams

Water splitting

A team of Italian scientists has created a sunlight-powered cell that produces pure hydrogen from water.

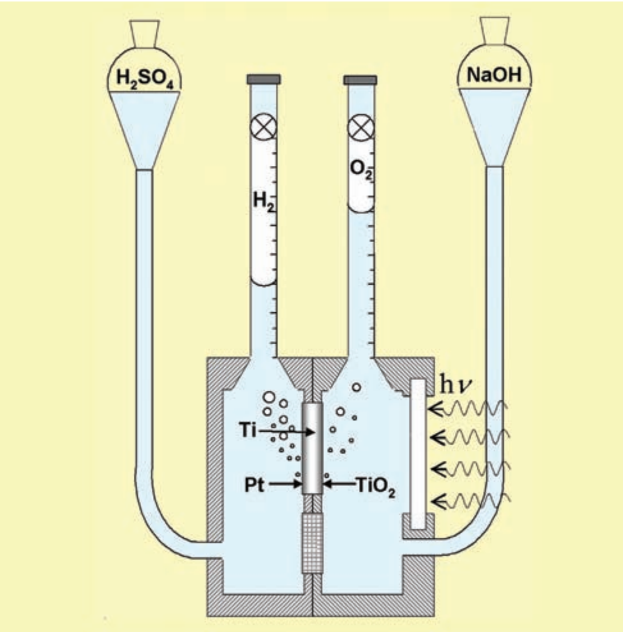
The team from the University of Milan and the University of Pavia are studying environmentally friendly ways to generate hydrogen, which could in future replace fossil fuels as a major energy source.

The new cell has two compartments filled with water and separated by an electrode made of platinum and titanium dioxide. When it is illuminated, by sunlight or an ordinary lamp, the electrode catalyses the splitting of the water into hydrogen and oxygen gas.

Elena Selli, who led the research, pointed out 'Almost all the photocatalytic water splitting systems described so far imply the evolution of a mixture of hydrogen and oxygen in only one reactor; of course, a separation step would be required prior to any use of hydrogen.' The new design of cell keeps the production of the two gases separate, resulting in streams of hydrogen and oxygen that do not need any purification to be useful.

'Our results demonstrate that hydrogen production from water photocatalytic splitting should be regarded as a practically viable, extremely promising way for clean, low cost and environmentally friendly conversion of solar energy into chemical energy,' said Selli. The team is working on improving the efficiency of the cell by making the titanium dioxide layer of the electrode more sensitive to visible light.

Clare Boothby



The two gases are produced from different sides of the membrane

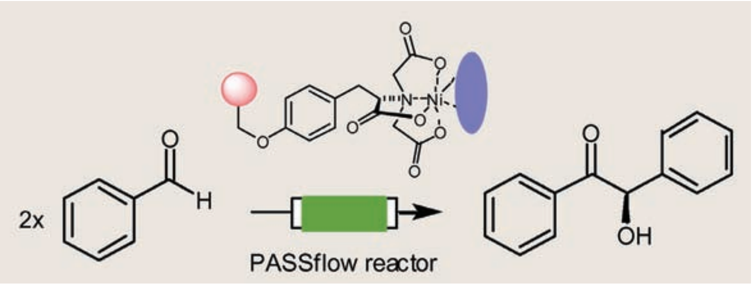
Reference

E Selli *et al*, *Chem. Commun.*, 2007, DOI: 10.1039/b711747g

---

Nickel ions used for simulataneous purification and immobilisation

Ready-to-use enzyme reactors within minutes



The enzymes (blue) are linked to the polymers (pink) by Ni-NTA

A fast multi-step microreactor for enzymatic synthesis has been developed by scientists in Germany.

The system has influences from both chemical synthesis and molecule biology according to its developers, Gerald Dräger and colleagues from University of Hannover in Leibniz. The new system enables both the immobilisation and purification of enzymes in the same reactor, which can then be used for a variety of enzymatic syntheses. Using this technique it is possible to obtain ready-to-use enzyme reactors from crude protein mixtures within minutes.

The system uses immobilised Ni-NTA (nitrilotriacetic acid) with a new tyrosine linker, attached to polymeric materials inside the reactor chamber. The reactor itself is integrated into an HPLC set-up. The NTA component is used in metal ion affinity chromatography, which in turn can be used to purify His6-tagged proteins from crude cell extracts. The polymeric materials in the reactor have also been altered to be more polar, ideal for biological molecules.

'The NTA linker is used to chelate with the Ni ion. The bound Ni ions themselves catch enzymes or proteins in the solution,' explained Dräger. This means that crude cell extracts can be both purified and immobilised simultaneously using this system, speeding up the whole process as normal reactors miss the purification step.

'The new tyrosine-based linker as compared to the standard lysine linker gives us higher loadings, increased efficiency and less purity problems,' added Dräger. The reactor system is flexible, meaning that different enzymes can be used. It also has the added advantages that it is licence-free and the reactor can be re-used a number of times.

Michele Zgraggen

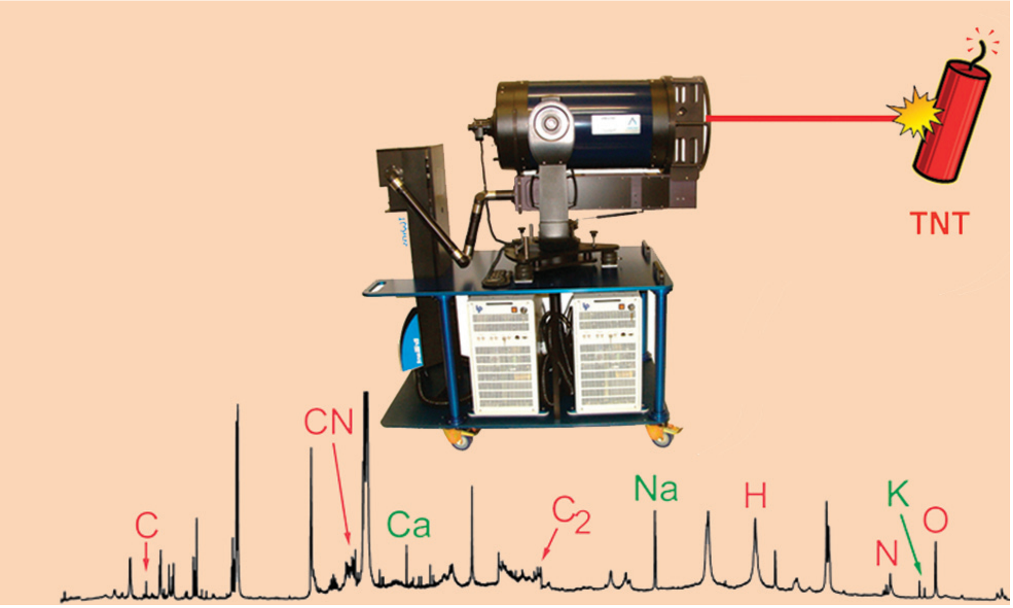
Reference

G Dräger *et al*, *Org. Biomol. Chem.*, 2007, **5**, 3657 (DOI: 10.1039/b712804e)

©The Royal Society of Chemistry 2007

Spectroscopy measures atomic ratios to find explosives

Detection at a distance



Chemistry is helping scientists in the US to detect explosives from a safer distance.

Detecting trace amounts of explosives from a distance quickly and accurately is a key aim for both the military and security sectors. Jennifer Gottfried and her team at the US Army Research Laboratory in Maryland have developed a detection system sensitive and selective enough to detect explosive residues at 20 m. Their system uses laser induced breakdown spectroscopy (LIBS) to identify molecules.

LIBS uses a laser pulse to turn a small part of a sample into a plasma of excited atoms and ions. As the plasma cools the characteristic atomic spectra of its constituents can be detected. The idea is that energetic molecules (potential explosives) contain higher ratios of oxygen and nitrogen to carbon and so can be identified by looking at the ratios of these atoms in a sample. This is far from straightforward, however, not least because nitrogen and oxygen are the main components of air.

Laser-induced breakdown spectroscopy looks at how much oxygen and nitrogen are present

Gottfried and her colleagues think they have overcome the problems. Using an argon flow to displace air reduced the interference from air sufficiently, but is impractical for detecting explosives at a distance. For this, they discovered that using a second laser pulse instead of only a single pulse enabled sufficient separation of the N and O peaks due to air from those of the sample compounds.

The team then developed suitable chemometric methods to enable interpretation of the data so that detection of energetic molecules was possible, even in the presence of interferences, such as dust.

Gottfried hopes these developments will fill an important gap in security systems. 'Currently there are no proven technologies that can accomplish residue explosives detection at a distance in a real-world scenario,' said Gottfried. She is optimistic that it will develop into a usable device, saying 'We expect that this technology will be available commercially very soon.'

Further development is still needed though, as Gottfried makes clear: 'This technology still needs to be verified and validated in real-world applications. We are moving in that direction.'

Edward Morgan

Reference

J L Gottfried *et al*, *J. Anal. At. Spectrom.*, 2008, DOI: 10.1039/b703891g

News in brief

Finding the right blend
Non-invasive infra-red spectrometry can provide scientists with improved quality checks for pharmaceutical production.

Cell culture and lysis on a chip is BASIC
US researchers have come up with a general strategy to integrate several biological steps in one microchip reactor.

See **www.rsc.org/chemicaltechnology** *for full versions of these articles*

This month in *Chemical Science*

Water – not just a solvent
Scientists in Germany have used water to improve the catalytic activity of coupling reactions making them greener and faster.

Pesticide persists in German rivers
Levels of the pesticide terbutryn in German rivers have not fallen, despite having been banned in 2003, say environmental researchers.

The changing colour of gold
DNA and gold nanoparticles provide a more sensitive way to detect copper ions in nature.

See **www.rsc.org/chemicalscience** *for full versions of these articles*

This month in *Chemical Biology*

Bringing warhead efficiency to light
US scientists can now compare molecular warheads that inactivate proteins.

Emotional enzymes
Chemists in the US have created fluorescent probes that can detect enzymes affecting our emotions.

Cells surface in semisynthesis
Scientists in Japan are using cells as protein factories

See **www.rsc.org/chembiology** *for full versions of these articles*

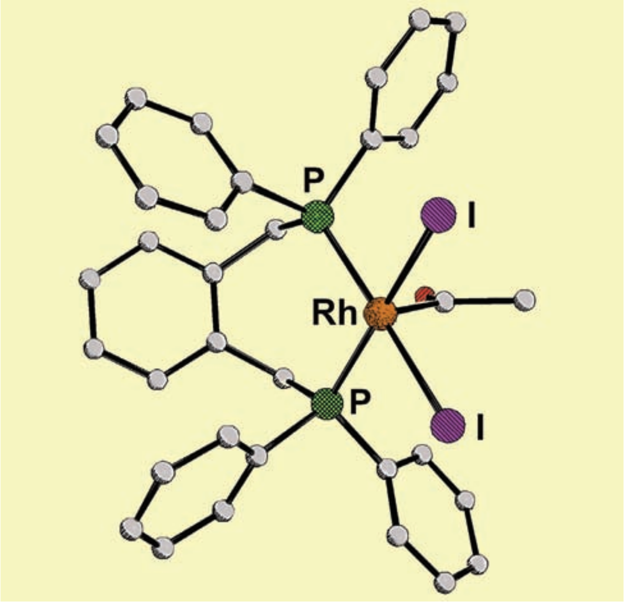
Selective ligand loves carbon monoxide, hates hydrogen

I capture the catalyst

The largest transition metal-catalysed process in the chemical industry could soon get an efficiency boost, thanks to the isolation of a key catalytic intermediate.

UK chemists have made a new series of catalysts in an effort to up the efficiency of one of the most widely used, and energy-intensive, catalytic processes in the chemical industry – the conversion of carbon monoxide (CO) and methanol into acetic acid. Matthew Clarke and colleagues at St Andrews University, UK, have examined a series of diphosphine ligands in the rhodium-catalysed carbonylation of methanol. 'This is one of the simplest organic reactions there is, but because of the scale, it must be done so incredibly efficiently,' said Clarke.

The industrial process used currently, BP's Cativa process, requires the starting CO to be purified, and the final product to be distilled – both of which are energy-expensive processes. Now BP is funding a project to look for the next generation of catalyst to get around either, or both, of these drawbacks.



The rhodium complex could cut out the purification step

Cheaper, lower grade CO includes large amounts of hydrogen, so to use it you need a catalyst that reacts with the CO but not the hydrogen, said Clarke. 'We identified a ligand, dppx [tetrakis(diphenylphosphino)-*p*-xylene], that was very selective,' he said. 'We isolated the catalytic intermediate, and showed it doesn't react with hydrogen, where the others do, so this is likely to be the origin of the selectivity.

'We're already making new catalysts based on this work, trying to gain a rational understanding of the selectivity,' Clarke added. 'We haven't cracked it yet, but I have an inkling there is a ligand out there that is active, selective, stable and commercially viable.'

Andreas Danopoulos, who studies catalysis at the University of Southampton, UK, said the work was a good approach to understanding the catalyst. 'But I'm not sure that rational design is the best way to solve this problem – I think a combinatorial approach [to screen a large number of possible ligands] would be better,' he said.

James Mitchell Crow

Reference
G Lamb *et al.*, *Dalton Trans.*, 2007 (DOI: 10.1039/b712974b)

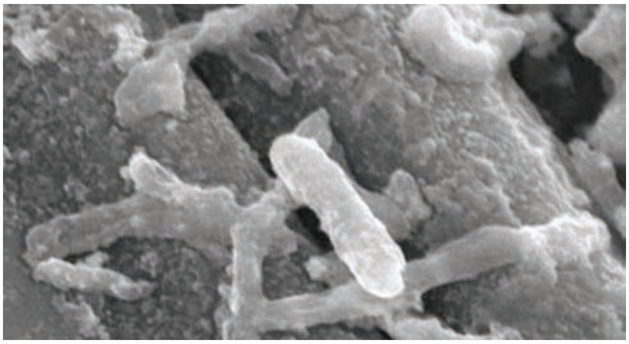
Microbes fuel the way to better water treatment

Bacteria act as miner's canary for toxins

Microbial fuel cells for detecting pollutant levels in wastewater have been developed by Korean scientists.

Hyung Joo Kim from Konkuk University, Seoul, and collaborators have developed fuel cells powered by bacteria for monitoring levels of toxins in water entering wastewater treatment plants.

Biological wastewater treatment plants rely on maintaining a carefully balanced mixture of bacteria and other organisms, said William Draper, an expert in environmental health from the Department of Health, California, US. He explained that effective methods are needed to monitor excessive levels of toxins in the water entering the plants so the organism balance can be maintained.



The fuel cell's output dips as toxins increase

The bacteria in Kim's fuel cells convert biochemical energy into electrical energy by oxidizing organic matter in the water. The electric current is then detected by a potentiometer, explained Kim. The bacteria generate a constant electric current under standard water pollutant levels. When the toxin levels in the water increase, however, the microbes become less efficient and electricity generation is inhibited. Draper likened this monitoring concept to 'the miner's canary'.

Further work is needed before these fuel cells can replace existing methods, explained Kim. He said that detection limits and specificity to various toxins need to be found, as well as ensuring the microbe community won't adapt to changes in pollutant levels.

Nina Athey-Pollard

Reference
M Kim *et al*, *J. Environ. Monit.*, 2007, DOI: 10.1039/b713114c

Interview

The fascination of catalysis

Ferdi Schüth talks to Madelaine Chapman about rockets, catalysis and law

Ferdi Schüth

Ferdi Schüth is a professor at the Max-Planck-Institut für Kohlenforschung in Mülheim an der Ruhr, Germany. His research focuses on the synthesis and characterisation of inorganic materials which have a use in catalysis. He is a member of the *Physical Chemistry Chemical Physics* advisory editorial board.

Who or what inspired you to become a scientist?

There was a fellow student in high school when I was 11 years old who went out after New Year, when we have rockets and fireworks in Germany, and collected the empty shells. We filled them with black powder and then tried to make them go again. We never got them to fly. They just exploded, but that was fun. Ever since then, I wanted to be a chemist.

How did you become interested in catalysis?

I wasn't interested in a particular topic so I selected an advisor to work with, who happened to do catalysis. For my habilitation, I worked with Professor Klaus Unger in Mainz, who is an inorganic chemist. I find this combination of inorganic/materials chemistry with catalysis really enjoyable. My career path involved many chance decisions which, in hindsight, turned out to be wonderful. Now I tell my students: 'don't plan too much.' My grandmother always said the one who plans early has to plan twice. There is a lot of wisdom in that.

What part of your research are you most proud of?

In 1992, I had an idea to stick a molecule into a zeolite channel. I proposed that if I had a single crystal of a zeolite, I should be able to analyse the orientation of the molecule in the zeolite with polarised infrared radiation using an infrared microscope. Infrared microscopes had just been introduced one year before. I wrote a proposal for this microscope which was granted. The very first day of experiments provided the spectra for a good paper. The fact that the idea immediately and directly worked made me very proud. Normally that never happens. Normally you have an idea but it fails and takes three times as long as you think.

I am also proud of a field we have developed over the last few years - the analysis of silicate species and the development of different species with mass spectrometry. This was much more complex and it certainly did not work straight away.

You are involved in the application of high-throughput experimentation to catalysis. How is this field progressing?

The field, which allows us to quickly screen a large number of catalysts, is pretty mature although it's only about 10 years old. The development of cutting-edge technology has moved into companies and is less of an academic topic nowadays. But there are still aspects of it where there are big challenges. In biotechnology, scientists do computational screening of molecule libraries. We would benefit greatly if we applied similar technology to materials science, especially catalysis. Even with the most powerful high-throughput techniques, it's not possible to explore all possible new catalysts experimentally. Developing computational methods to narrow down the search is one of the biggest challenges we have.

Can these techniques be used to gain physical insight into what's actually happening in a catalytic reaction?

Absolutely. Normally if we want to get insight, we measure the performance of different catalysts, we analyse catalyst composition, structure and so on and then we build models and try to derive structure-activity relationships. Thanks to high-throughput experimentation, we have more catalysts and more characterisation data and so the database from which we are establishing these relationships is a much wider one. Consequently, we can either get insight into these structure-activity relationships more quickly or we can get deeper insight because we see more.

What is the secret to running a successful research group?

My belief is that people working with me should have freedom. They have to think for themselves. I also strongly believe that people have to have fun at work. They have to like what they are doing. When I hire new people I am always looking for a fire burning in them. They need to be fascinated by the chemistry. I also think you need material resources. You can only go so far with just ideas - at some point you need steel and glass.

If you weren't a scientist, what would you do?

I would probably be a judge. I have both a law degree and a chemistry PhD. I had several different career possibilities - industrial chemist, patent lawyer, academic or judge - and I weighed up all their pros and cons. The ones that scored highest were an academic chemist and a judge in administration law.

©The Royal Society of Chemistry 2007

ACS and RSC:
Building the Future,
one molecule at a time.

The American Chemical Society and Royal Society of Chemistry are not-for-profit society publishers. We support excellence in research and education by investing in our future generations of chemists.

ACS PUBLICATIONS
HIGH QUALITY. HIGH IMPACT.
RSCPublishing

Instant insight

Holographic data storage

Avtar Matharu and colleagues from the University of York, UK, explain how, when it comes to data, size matters

Modern-day society lives in an information-obsessed world. The volume of information produced and stored annually is exponential in growth. The information age has arrived in all its glory with on-line access to vast resources of electronic information never imagined less than one decade ago. On a daily basis we are bombarded with high resolution digitised images utilising mega- and giga-bytes of information. In the area of home entertainment we can now purchase the latest state-of-the-art BluRay DVD player capable of storing a staggering 27 GB, surpassing its counterparts, the CD (750 MB or 75 minutes of music) and DVD (4.7 GB or a 2 hour movie). However, this is still not enough as the societal needs of the 21st century for increased information content with even faster processing speeds continue to grow at breakneck speed.

There's one big problem – storage space. Although magnetic disk is still the best medium for storage of large amounts of information, it has severe limitations. Magnetic disk, and conventional magneto-optical data storage technology, use the surface of the medium to store and retrieve bits of data. The available area on a magnetic disk cannot be compressed indefinitely to record even smaller bits of information due to the superparamagnetic effect. The diameter of the magnetic domains is limited to around 10 nm: smaller than this and thermal self-erasure occurs. The magnetised bit flips randomly, finding it difficult to attain a stable state.

New, alternative technologies need to be considered. Holography, an optical 3-D volumetric approach, may be the answer to meet the societal needs of the 21st century rather than the current 2-D surface approach. The concept of holography was first introduced by Gabor in 1948 but remained dormant for many years due to a lack of technological advances in complementary optics and image processing instrumentation. Holographic storage provides the potential to store in excess of one terabyte of information with transfer rates exceeding 1 GB/s and data access time of less than 100 µs.

In holographic storage, a whole page of information in the form of a bit-map is recorded at once, instead of storing single bits as in digital storage. Typically, two laser beams derived from a single laser source are overlapped on a photosensitive material. One of the beams, called the object beam, passes through the object (bit-map) of interest, and the other beam is a plane wave providing a phase reference. In conventional holography, the two beams have the same polarization. They create a complicated interference pattern in the film that is characteristic of the object. The recorded information is read out with a conjugate of the reference wave. By the process of angular multiplexing several holograms can be recorded in the same volume.

The world's information could be stored and retrieved within a liquid crystal holographic box

Significant advances have been made in holography, as exemplified by InPhase Technologies' tapestry™ holographic media, capable of storing and retrieving 200 GB on a standard 120 mm CD format at high speed, equivalent to a near ten-fold improvement on optical BluRay DVD technology. There are still drawbacks, however, as the ideal material is still to be found. Any material suitable for holographic storage should possess fast optical switching between two states, high thermal stability over a wide temperature range and non-destructive read-out. As the search for holographic materials continues, liquid crystals may play an important role. Liquid crystals constitute the fourth state of matter intermediate between the solid and the liquid states. The intermediate ordering of molecules between order and disorder may enhance storage properties. Although liquid crystals are not a pre-requisite for holographic storage, their anisotropic shape is important.

Imagine one day we may all be carrying a credit card with a 1 × 1 cm square hologram capable of storing all our personal details including medical records with X-ray scans. In the event of sudden serious illness the hologram may be read immediately to display your full medical history rather than having to wait for information to be sent by email or post. The time saved may ultimately save your life.

Reference

A S Matharu, S Jeeva and P S Ramanujam, *Chem. Soc. Rev.*, 2007, DOI: 10.1039/b706242g

Read the full Tutorial Review 'Liquid crystals for holographic optical data storage' in Issue 12 of Chemical Society Reviews.

©The Royal Society of Chemistry 2007

Essential elements

New RSC Books website

The RSC Books website has recently undergone a substantial revamp, and we are pleased to present our new and improved site. New features include improved functionality that allows users to browse RSC books by series, subject area, publication copyright year and by A–Z title searching. Alternatively, keyword or author searches can now be carried out using the built-in Google search. Forty years of RSC books are included on the new website, from early titles in 1968 to the books RSC will be publishing next year in 2008.

The new RSC Books website site is closely linked to our online shop with direct links to the RSC eBook Collection. This enhanced visibility enables you to view the table of contents and first chapter of any book in the collection free of charge. The new RSC Books website provides all the browser requirements, such as a shopping cart facility with selected special discounts function, needed for simple website navigation and ease of use. All the latest information can be found in the new RSC Books website: how to publish your book with RSC Publishing, titles in our RSC eBook Collection and regular website updates on our new releases, most popular titles and books for students.

For more information visit www.rsc.org/books

Tokeshi wins Pioneers in Miniaturisation prize

Manabu Tokeshi has been named as the 2007 winner of the Pioneers in Miniaturisation prize.

The prize, first awarded in 2006, was established by two of the major players in the miniaturisation sector, *Lab on a Chip* and Corning Incorporated.

Joydeep Lahiri, research director at Corning Inc., commented 'Tokeshi's multi-disciplinary research exemplifies the essential outreach that is necessary – particularly to the molecular biology or medical areas – in order to find "the next big thing" that will succeed, for example, Corning's μPlate technology.'

The prize aims to promote miniaturisation through micro and nanotechnologies to the wider scientific community and encourage both young and new scientists into the field.

From left: Harp Minhas, editor, *Lab on a Chip*; Manabu Tokeshi (2007 Award Winner); Joydeep Lahiri, research director, Corning Inc.; and Andreas Manz, chair of the *Lab on a Chip* editorial board.

Yoshinobu Baba of the Plasma Nanotechnology Research Center Nagoya University, Japan, said 'Tokeshi has been the powerhouse behind many interdisciplinary publications as his record shows.'

The presentation of this prestigious award was made at the μTAS 2007 conference held in Paris, France, in October.

For more information see www.rsc.org/loc

And finally...

***Molecular BioSystems* unzips ...**
From January 2008 *Molecular BioSystems* will form its very own strand of science as a stand alone monthly journal, becoming solely available to readers and subscribers independently of its host journal. Read more on how the journal is serving the community and why it is ready to unzip at *www.molecularbiosystems.org*

Speaking volumes...
Times flies when you're publishing high impact science. In 2008, four RSC journals celebrate their tenth year of publication: *Physical Chemistry Chemical Physics*, *CrystEngComm*, *Green Chemistry* and the *Journal of Environmental Monitoring*. These diverse journals are all now firmly established as market leaders in their subject areas, with each continuing to go from strength to strength. Watch out for special 10th anniversary events and celebrations throughout 2008!

Chemical Technology (ISSN: 1744-1560) is published monthly by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge UK CB4 0WF. It is distributed free with *Chemical Communications, Journal of Materials Chemistry, The Analyst, Lab on a Chip, Journal of Environmental Monitoring, Green Chemistry, CrystEngComm, Physical Chemistry Chemical Physics* and *Analytical Abstracts*.
Chemical Technology can also be purchased separately. 2007 annual subscription rate: £199; US $376. All orders accompanied by payment should be sent to Sales and Customer Services, RSC (address above). Tel +44 (0) 1223 432360, Fax +44 (0) 1223 426017 Email: sales@rsc.org

Editor: Neil Withers

Associate editors: Nicola Nugent, Celia Clarke

Interviews editor: Joanne Thomson

Essential Elements: Daniel Bradnam, Rebecca Jeeves, and Kathryn Lees

Publishing assistant: Ruth Bircham

Publisher: Graham McCann

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the copyright and Related Rights Regulations 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission of the Publisher or in the case or reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK.
US copyright law is applicable to users in the USA.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions.

Royal Society of Chemistry: Registered Charity No. 207890.

RSC Publishing

©The Royal Society of Chemistry 2007